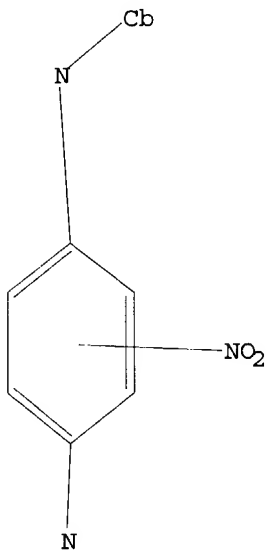
> d his

(FILE 'HOME' ENTERED AT 08:55:47 ON 08 JUL 2004)

FILE 'REGISTRY' ENTERED AT 08:55:52 ON 08 JUL 2004
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 22 S L1 FUL

FILE 'CAPLUS' ENTERED AT 08:56:31 ON 08 JUL 2004
L4 10 S L3

=> d l1
L1 HAS NO ANSWERS
L1 STR

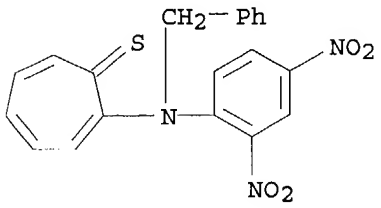


Structure attributes must be viewed using STN Express query preparation.

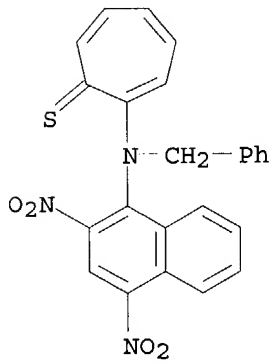
=> d bib abs hitstr 1-10

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:599224 CAPLUS
DN 138:136761
TI Acylotropic Tautomerism: XXXV. R.dblarw.L-Inversion of Configuration of Dipolar Spyrocyclic and Open-Chain 2-Arylaminotropone Isomers
AU Olekhnovich, L. P.; Budarina, Z. N.; Borodkin, G. S.; Kurbatov, S. V.; Vaslyaeva, G. S.; Zhdanov, Yu. A.
CS Rostov State University, Rostov-on-Don, 344090, Russia
SO Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (2002), 38(5), 713-722
CODEN: RJOCEQ; ISSN: 1070-4280
PB MAIK Nauka/Interperiodica Publishing
DT Journal
LA English
OS CASREACT 138:136761
AB R.dblarw.L-Inversion of chiral spirocyclic and open-chain 2-arylaminotropone derivs. with varied heteroatom (O, S, N) was studied. Kinetic relations holding in the RL-permutation are discussed. Its mechanism includes formation and dissociation of spiro bonds and torsion stereodynamics.

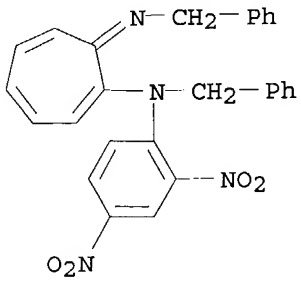
IT **491879-87-9**
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(acylotropic tautomerism and R.dblarw.L-inversion of configuration of dipolar spirocyclic and open-chain 2-arylaminotropone isomers)
RN 491879-87-9 CAPLUS
CN 2,4,6-Cycloheptatriene-1-thione, 2-[(2,4-dinitrophenyl)(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



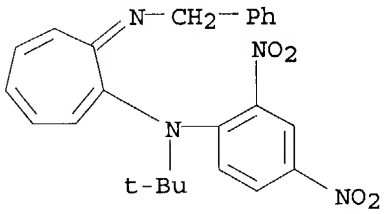
IT **491879-88-0**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(acylotropic tautomerism and R.dblarw.L-inversion of configuration of dipolar spirocyclic and open-chain 2-arylaminotropone isomers)
RN 491879-88-0 CAPLUS
CN 2,4,6-Cycloheptatriene-1-thione, 2-[(2,4-dinitro-1-naphthalenyl)(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



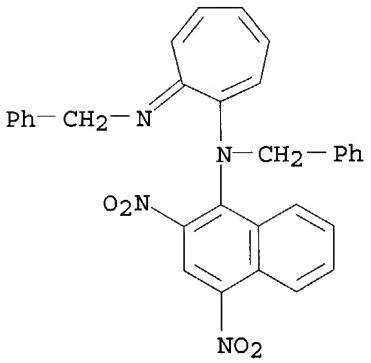
IT **491879-82-4P 491879-83-5P 491879-84-6P**
491879-89-1P 491879-94-8P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(acylotropic tautomerism and R.dblarw.L-inversion of configuration of dipolar spirocyclic and open-chain 2-arylaminotropone isomers)
RN 491879-82-4 CAPLUS
CN 1,3,5-Cycloheptatrien-1-amine, N-(2,4-dinitrophenyl)-N-(phenylmethyl)-7-[(phenylmethyl)imino]- (9CI) (CA INDEX NAME)



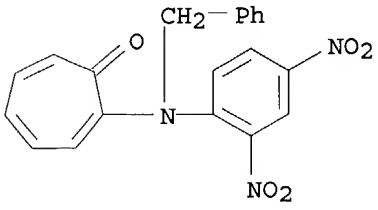
RN 491879-83-5 CAPLUS
CN 1,3,5-Cycloheptatrien-1-amine, N-(1,1-dimethylethyl)-N-(2,4-dinitrophenyl)-7-[(phenylmethyl)imino]- (9CI) (CA INDEX NAME)



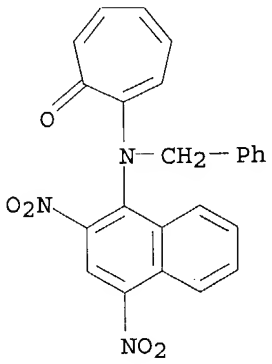
RN 491879-84-6 CAPLUS
CN 1-Naphthalenamine, 2,4-dinitro-N-(phenylmethyl)-N-[7-[(phenylmethyl)imino]-1,3,5-cycloheptatrien-1-yl]- (9CI) (CA INDEX NAME)



RN 491879-89-1 CAPLUS
CN 2,4,6-Cycloheptatrien-1-one, 2-[(2,4-dinitrophenyl)(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

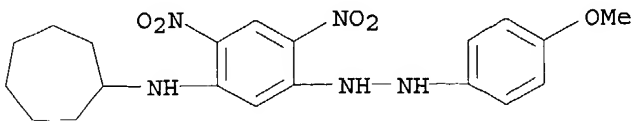


RN 491879-94-8 CAPLUS
CN 2,4,6-Cycloheptatrien-1-one, 2-[(2,4-dinitro-1-naphthalenyl)(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

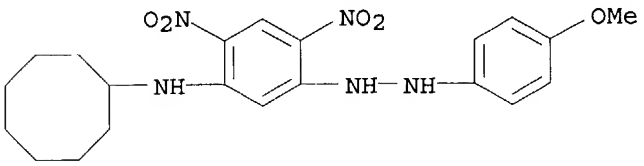


RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:924420 CAPLUS
DN 136:162487
TI Identification of Novel Ah Receptor Agonists Using a High-Throughput Green Fluorescent Protein-Based Recombinant Cell Bioassay
AU Nagy, Scott R.; Liu, Gang; Lam, Kit S.; Denison, Michael S.
CS Department of Environmental Toxicology, University of California, Davis, CA, 95616, USA
SO Biochemistry (2002), 41(3), 861-868
CODEN: BICHAW; ISSN: 0006-2960
PB American Chemical Society
DT Journal
LA English
AB The Ah receptor is a ligand-dependent transcription factor that mediates the biol. and toxic effects of polycyclic aromatic hydrocarbons and halogenated aromatic hydrocarbons such as 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD, dioxin). Recent evidence also suggests a role for the AhR in normal physiol. and development. Although a variety of structurally diverse chems. are reported to bind to and activate the AhR, the full spectrum of structural chemical classes that can interact with the AhR remains to be elucidated. Large-scale anal. of the ligand binding specificity of the AhR requires the use of a high-throughput AhR bioassay system for chemical screening. We have utilized a recombinant mouse hepatoma cell line (H1G1.1c3) containing a stably integrated TCDD- and AhR-responsive enhanced green fluorescent protein (EGFP) reporter gene to screen a 1,5-dialkylamino-2,4-dinitrobenzene combinatorial chemical library consisting of 155 parental amines and up to 12 090 combinatorial products in less than 7 days for novel AhR agonists. These analyses have identified numerous parental amines as relatively potent inducers of EGFP (with EC50s between 8 and 1000 μM) and also have revealed several novel products of the combinatorial chemical library synthesis with EC50s between 10 and 100 μM. Overall, these results have not only allowed the identification of novel activators of the AhR but also demonstrate the utility of the recombinant H1G1.1c3 cell bioassay for high-throughput chemical screening.
IT **396992-80-6P 396993-01-4P**
RL: BSU (Biological study, unclassified); CPN (Combinatorial preparation); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation)
(identification of novel Ah receptor agonists using high-throughput green fluorescent protein-based recombinant cell bioassay)
RN 396992-80-6 CAPLUS
CN Cycloheptanamine, N-[5-[2-(4-methoxyphenyl)hydrazino]-2,4-dinitrophenyl]- (9CI) (CA INDEX NAME)



RN 396993-01-4 CAPLUS
CN Cyclooctanamine, N-[5-[2-(4-methoxyphenyl)hydrazino]-2,4-dinitrophenyl]-(9CI) (CA INDEX NAME)

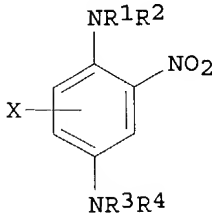


RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:207825 CAPLUS
DN 134:242400
TI Hair coloring preparations based on 2-nitro-p-phenylene-derivative direct dyes
IN Naumann, Frank; Rose, David; Meinigke, Bernd; Hoeffkes, Horst
PA Henkel K.-G.a.A., Germany
SO Ger. Offen., 10 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19944528	A1	20010322	DE 1999-19944528	19990917
	WO 2001021144	A2	20010329	WO 2000-EP8774	20000908
	WO 2001021144	A3	20011011		
	W: AU, JP, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	EP 1212032	A2	20020612	EP 2000-971277	20000908
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
PRAI	DE 1999-19944528	A	19990917		
	WO 2000-EP8774	W	20000908		

OS MARPAT 134:242400
GI



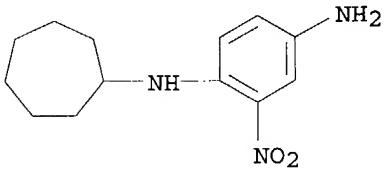
I

AB The invention concerns hair coloring formulations that contain only direct dyes and at least one of the dyes is a 2-nitro-p-phenylene-derivative (I),

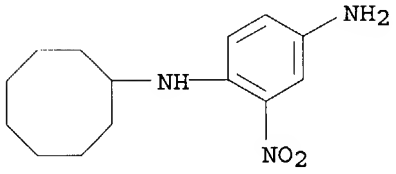
where R1-R4 = H, C1-C4 hydroxyalkyl, C7 or C8-ring saturated, unsatd., substituted and at least one of R1-R4 is from the C7 or C8-ring group; X = H, halogen; the dyes shift the color to read. The compns. further include developers, coupling agents and can also include other direct dyes. The compns. do not contain oxidative dye precursors. Thus 1-(N-cycloheptylamino)-4-amino-2-nitrobenzene was prepared and used in a two-component composition It was used in component B along with (in g) ammonium sulfate 1, water to 100, ammonia to pH = 9. Component A contained in g: cetearyl alc. 1.00; coco fatty alcs. 1.00; Akypo RLM45N 1.10; p-hydroxybenzoic acid Pr ester 0.05; p-hydroxybenzoic acid Me ester 0.15; water to 70.

IT **330456-77-4P 330456-78-5P**
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(hair coloring prepns. based on 2-nitro-p-phenylene-derivative direct dyes)

RN 330456-77-4 CAPLUS
CN 1,4-Benzenediamine, N1-cycloheptyl-2-nitro- (9CI) (CA INDEX NAME)



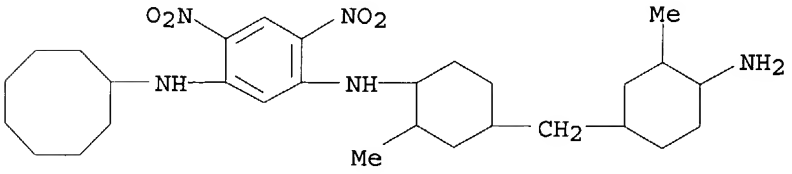
RN 330456-78-5 CAPLUS
CN 1,4-Benzenediamine, N1-cyclooctyl-2-nitro- (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:532245 CAPLUS
DN 133:281562
TI Solution-Phase Synthesis of a 1,5-Dialkylamino-2,4-dinitrobenzene Library and the Identification of Novel Antibacterial Compounds from This Library
AU Liu, Gang; Fan, Yemei; Carlson, James R.; Zhao, Zhan-Gong; Lam, Kit S.
CS Department of Internal Medicine UC Davis Cancer Center and Department of Pathology, UC Davis Medical Center, Sacramento, CA, 95817, USA
SO Journal of Combinatorial Chemistry (2000), 2(5), 467-474
CODEN: JCCHFF; ISSN: 1520-4766
PB American Chemical Society
DT Journal
LA English
OS CASREACT 133:281562
AB A small mol. library containing 1,5-dialkylamino-2,4-dinitrobenzene derivs. can be generated by a highly efficient solution-phase synthesis method. From this 2485-member library, a series of novel compds. with antibacterial activity were isolated. The significance of this report is that the synthetic scheme is extremely simple, with minimal number of liquid handling steps, and the solvents and reagents left in the final library preparation are fully compatible with cell-based assays.

IT **299899-35-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological

study); PREP (Preparation)
(solution-phase preparation of dinitrobenzenediamine combinatorial library and
identification of antibacterial compds.)
RN 299899-35-7 CAPLUS
CN 1,3-Benzenediamine, N-[4-[(4-amino-3-methylcyclohexyl)methyl]-2-methylcyclohexyl]-N'-cyclooctyl-4,6-dinitro- (9CI) (CA INDEX NAME)

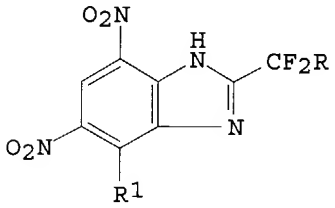


RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:140050 CAPLUS
DN 86:140050
TI 4-Substituted-5,7-dinitro-2-(α,α-difluoroalkyl)-benzimidazole compounds as insecticides
IN Miesel, John L.
PA Eli Lilly and Co., USA
SO U.S., 23 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4000295	A	19761228	US 1975-588972	19750620
	US 3790595	A	19740205	US 1972-221809	19720128
PRAI	US 1969-833685		19690616		
	US 1972-221809		19720128		
	US 1973-415100		19730910		

GI



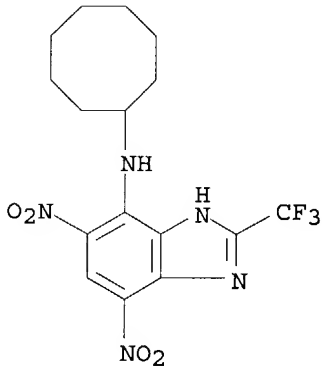
I

AB Benzimidazoles I (R = F, Cl, CF3, CF2CF3; R1 = alkylthio, alkoxy, alkyl, NR2R3, R2 = H, R3 = alkyl, cycloalkyl; R2 = R3 = alkyl, cycloalkyl; NR2R3 = piperidino, octaazocino, decaisoquinolyl, hexaazepino, azabicycloalkanyl) (106 compds.) were prepared Thus, I (R = F, R1 = Cl) (II) was treated with Me3CNH2 in the presence of Et3N to give I (R = F, R1 = Me3CNH). Similar treatment of II with piperidine gave I (R = F, R1 = piperidino). The reaction of cyclohexanol and K and II in PO(NMe2)3 gave I (R = F, R1 = cyclohexyloxy) and of EtCHMeSNa and II gave I (R = F, R1 = EtCHMeS). These I exhibited insecticidal activity against the Mexican bean beetle, southern armyworm, the two-spotted spider mite, milkweed bug, house fly, and the boll weevil.
IT **30542-91-7P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and insecticidal activity of)

RN 30542-91-7 CAPLUS

CN 1H-Benzimidazol-4-amine, N-cyclooctyl-5,7-dinitro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

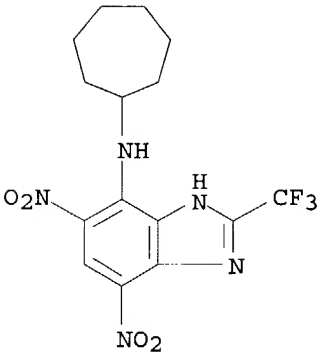


IT **30542-96-2P 30548-48-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

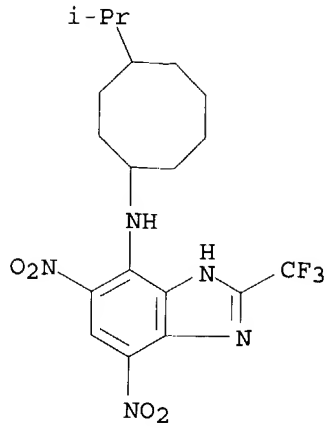
RN 30542-96-2 CAPLUS

CN 1H-Benzimidazol-4-amine, N-cycloheptyl-5,7-dinitro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 30548-48-2 CAPLUS

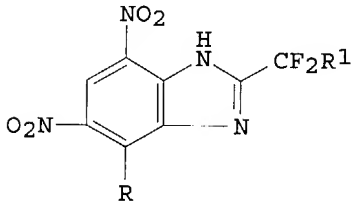
CN 1H-Benzimidazol-4-amine, N-[4-(1-methylethyl)cyclooctyl]-5,7-dinitro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:494361 CAPLUS
DN 85:94361
TI 4-Substituted-5,7-dinitro-2-(α,α-difluoroalkyl)benzimidazole compounds
IN Miesel, John L.
PA Eli Lilly and Co., USA
SO U.S., 21 pp. Division of U.S. 3,790,595.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3927020	A	19751216	US 1973-415099	19730910
	US 3790595	A	19740205	US 1972-221809	19720128
PRAI	US 1969-833685		19690616		
	US 1972-221809		19720128		

GI

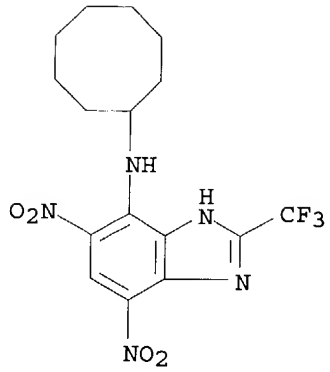


I

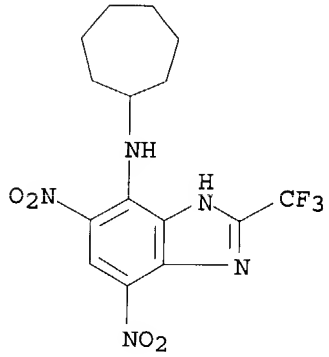
AB About 130 benzimidazoles I (R = Me3CNH, Me2CHCH2CHMeN, piperidino, Me3CS, cyclohexyloxy, PrNH, BuNEt, MeO, MeS, etc.; R1 = F, Cl, CF3) were prepared by treating I (R = Cl) with RH. I [R = Me(CH2)4, R1 = F] was prepared by treating I (R = Cl) with BuCH(CO2Et)2 followed by hydrolysis and decarboxylation. At 50 ppm I (R = Me2CHCH2CMeNH, R1 = F) controlled 91-100% Mexican bean beetle.

IT **30542-91-7P 30542-96-2P 30548-48-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

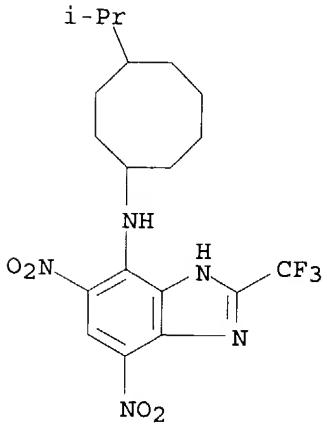
RN 30542-91-7 CAPLUS
CN 1H-Benzimidazol-4-amine, N-cyclooctyl-5,7-dinitro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 30542-96-2 CAPLUS
CN 1H-Benzimidazol-4-amine, N-cycloheptyl-5,7-dinitro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

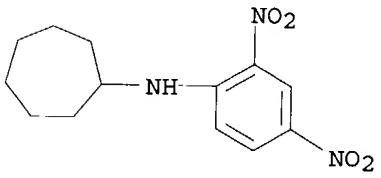


RN 30548-48-2 CAPLUS
CN 1H-Benzimidazol-4-amine, N-[4-(1-methylethyl)cyclooctyl]-5,7-dinitro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

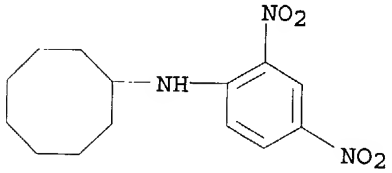


L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1971:111632 CAPLUS
DN 74:111632
TI Cycloalkylsulfamic acids and their salts
AU Unterhalt, Bernard; Boeschemeyer, L.
CS Inst. Pharm. Chem. Lebensmittelchem., Univ. Marburg/Lahn, Marburg/Lahn,

Fed. Rep. Ger.
SO Zeitschrift fuer Lebensmittel-Untersuchung und -Forschung (1971), 145(2), 93-6
CODEN: ZLUFAR; ISSN: 0044-3026
DT Journal
LA German
AB Cycloalkylsulfamic acids, their salts, N,N'-dicycloalkylsulfamides, and (dinitrophenyl)amines were prepared from cycloalkylamines. The sweetness of the unsubstituted Na cycloalkylsulfamates was tested.
IT **31846-31-8P 31846-32-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 31846-31-8 CAPLUS
CN Cycloheptylamine, N-(2,4-dinitrophenyl)- (8CI) (CA INDEX NAME)



RN 31846-32-9 CAPLUS
CN Cyclooctylamine, N-(2,4-dinitrophenyl)- (8CI) (CA INDEX NAME)



L4 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1971:53792 CAPLUS
DN 74:53792
TI Insecticidal 4-amino-5,7-dinitro-2-(trifluoromethyl)benzimidazoles
IN Miesel, John L.
PA Eli Lilly and Co.
SO Ger. Offen., 64 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 3

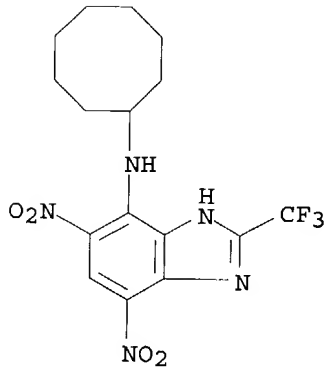
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2029753	A	19701217	DE 1970-2029753	19700616
	ES 380609	A1	19730401	ES 1970-380609	19700610
	GB 1272208	A	19720426	GB 1970-1272208	19700615
	FR 2052666	A5	19710409	FR 1970-22123	19700616
	JP 49016938	B4	19740425	JP 1970-52332	19700616
	CH 554345	A	19740930	CH 1970-9108	19700616
PRAI	US 1969-833685		19690616		

GI For diagram(s), see printed CA Issue.
AB The title compds. (I) were prepared from the 4-chloro compound with RR1NH. I were used against various insects, e.g. Mexican bean beetle (Epilachna varivestis), boll weevil (Anthonomus grandis), housefly, southern armyworm (Prodenia eridania) and milkweed bug (Oncopeltis fasciatus), and mites, e.g. red spider mites. Among .apprx.50 I prepared were (R and R1 given): tert-Bu, H; Pr, Me; Bu, Bu; CH2C.tplbond.CH, H; CH2CF3, H; cyclopropyl, H;

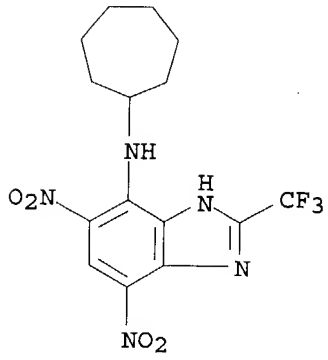
(NRR1 =) piperidino, decahydro-1-quinolyl.

IT **30542-91-7P 30542-96-2P 30548-48-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

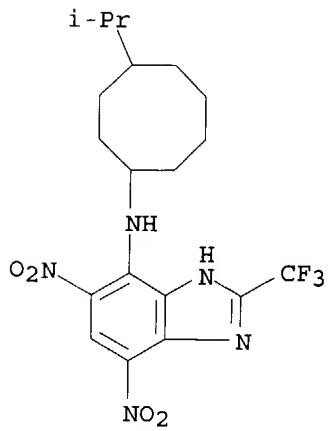
RN 30542-91-7 CAPLUS
CN 1H-Benzimidazol-4-amine, N-cyclooctyl-5,7-dinitro-2-(trifluoromethyl)-(9CI) (CA INDEX NAME)



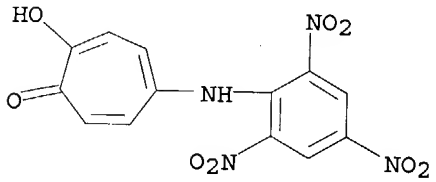
RN 30542-96-2 CAPLUS
CN 1H-Benzimidazol-4-amine, N-cycloheptyl-5,7-dinitro-2-(trifluoromethyl)-(9CI) (CA INDEX NAME)



RN 30548-48-2 CAPLUS
CN 1H-Benzimidazol-4-amine, N-[4-(1-methylethyl)cyclooctyl]-5,7-dinitro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1963:54865 CAPLUS
DN 58:54865
OREF 58:9420e-g
TI Effects of chemicals on the mitotic cell in plant, with special reference to tropoids
AU Shimizu, Yoshitaka
CS Tohoku Univ., Sendai, Japan
SO Sci. Rept. Tohoku Univ., Fourth Ser. (1962), 28, 143-78
DT Journal
LA English
AB The relation between chemical structure and toxicity to cell division, for more than 100 compds., mostly with an unsatd. 7-C ring as colchicine, were studied for induction of mitotic abnormalities. The compds. were dissolved in a water-miscible solvent and next diluted with water to make 0.1, 0.01, 0.001, and 0.0001% solns. Various meristematic tissues from Allium cepa, Tradescantia pcludosa, and Vicia faba were incubated in these solns. during 4 and 24 hrs. at 22°. Squash prepns. were fixed with a Carnoy 3:1 solution, stained with Feulgen reagent together with an aceto-orcein staining, if necessary, and examined for mitotic aberrations, 11 types of which were distinguished. The toxicity of such mitotic poisons as N-mustard compds. can be increased by replacing their benzene ring by the unsatd. 7-C ring. This ring itself is not essential for mitotic toxicity, but rather its flatness and (or) the π-electron polarity is related with this toxicity. Hydrophilic properties from heterocyclic 5-membered rings containing N or S promote binucleate cell formation by phragmoplast disturbance. Especially side chain radicals induce chromosome denaturation, the order of toxicity being OCH3 < OH < NH2. Such induction of mitotic activity in mature tissue as exerted by plant growth substances is shown by some monoazaazulene derivatives.
IT **91805-09-3**, 2,4,6-Cycloheptatrien-1-one, 2-hydroxy-5-(2,4,6-trinitroanilino)-
(plant cell division response to)
RN 91805-09-3 CAPLUS
CN 2,4,6-Cycloheptatrien-1-one, 2-hydroxy-5-(2,4,6-trinitroanilino)- (7CI) (CA INDEX NAME)



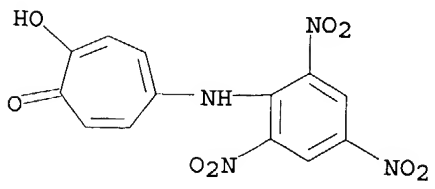
L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1952:45329 CAPLUS
DN 46:45329
OREF 46:7560h-i,7561a-e
TI Tropolone derivatives. X. p-Aminotropolone. II
AU Nozoe, Tetsuo; Seto, Shuichi; Ito, Sho; Sato, Masatsune
CS Tohoku Univ., Sendai
SO Proc. Japan Acad. (1951), 27, 426-9
DT Journal
LA Unavailable
AB cf. C.A. 46, 962g. 5-Aminotropolone (I) in EtOH with Br gives no crystalline product, but similar treatment of 5-acetamidotropolone gives a mono-Br compound (II), m. 201-4°, analyzing for an ethanolate, C9H8O3NBr.EtOH. II with Ac2O gives a di-Ac derivative (III), m. 166-7°, undepressed by mixture with the diacetate of 5-amino-3-bromotropolone, obtained earlier from 3-bromotropolone via an

azo compound Bromination of the di-Ac derivative of I also yields III. I, its mono- and di-Ac derivs., and its Me ether give only intractable materials on treatment with 1 or 2 equivs. HNO3 in HOAc or concentrated H2SO4. The Schotten-Baumann reaction converts I to 5-benzamidotropolone, colorless scales, m. 181-2°. I does not condense easily in EtOH-HOAc with benz-, salicyl-, or anisaldehydes or with vanillin, but p-O2NC6H4CHO gives a p-nitrobenzylidene derivative, m. 202-4° (decomposition), which is H2O-insol., easily hydrolyzed by hot H2O, and gives a red color with FeCl3. Diazotization of I in concentrated H2SO4, followed by dilution with H2O and heating to 80°, yields 5-hydroxytropolone (IV), yellow needles, m. 251° (decomposition) (blackens at 245°), soluble in Me2CO, EtOH, and HOAc, insol. in C6H6 and Et2O, and sublimes at 5 mm. and 170-80°; it gives a H2O-insol. yellow Na salt, a purple-black ferric complex salt, and a yellow Cu complex salt. These salts melt above 350°. Heating IV with Ac2O, followed by treatment with H2O, gives a monoacetate, yellow scales, m. 87-8°, which turns red when treated with FeCl3. When diazotized in EtOH, then heated to 70°, I gives 5-ethoxytropolone, colorless needles, m. 135-5.5°, soluble in Me2CO, EtOH, C6H6, and Et2O but insol. in petr. ether; its Na salt is yellow, its Cu complex yellow-green, and its FeCl3-reaction product red-orange. The preparation of 5-chlorotropolone, m. 181-5.3°, and of 5-iodotropolone, m. 185-6°, from I via Sandmeyer reactions has been reported in an earlier paper (loc. cit.), but the m.ps. cited there are in error. I in EtOH with PhNCS gives 5-(3-phenyl-2-thioureido)tropolone (1-phenyl-3-(5-tropolonyl)-2-thiourea), yellow prisms, m. 150-1° (decomposition). I and p-AcNHC6H4SO2Cl in pyridine give 5-(p-acetamidophenylsulfonamido)tropolone, yellow needles, m. 224-5° (decomposition). With MeI and K2CO3 in MeOH solution, I yields pale yellow scales, m. 215-18°, presumed to be 5-(dimethylamino)tropolone-MeI (5-tropolonyltrimethylammonium iodide). Picryl chloride and I in MeOH containing NaOAc yield 5-(picrylamino)tropolone, red-orange scales, m. 249-51° (decomposition). I did not react with urea, nitrourea, CS2, or dicyandiamide. Aqueous solns. of the alkali-metal salts of I rapidly turn red-brown in air. Evaporation of a solution of I in excess HCl to a small volume gives a compound 2I.3HCl (V), m. 223-4° (decomposition). V with KSCN gives yellow needles, 2I.HSCN.H2O, m. 128-30°. Aqueous solns. of the Na salt of I treated with HCl to pH 5 yield crystals, I.HCl.H2O, m. 115-17°, a 2nd crystalline substance, m. 180-5°, of unknown composition The behavior of I differing from that of ordinary arylamines (low yields of halo and HO derivs., difficult condensation with aryl aldehydes to give products more easily hydrolyzed, poor reaction with urea, etc.) is attributed to resonance and tautomeric structures tending to decrease the basicity of the NH2 group.

IT **91805-09-3**, 2,4,6-Cycloheptatrien-1-one, 2-hydroxy-5-(2,4,6-trinitroanilino)-
(preparation of)

RN 91805-09-3 CAPLUS

CN 2,4,6-Cycloheptatrien-1-one, 2-hydroxy-5-(2,4,6-trinitroanilino)- (7CI) (CA INDEX NAME)



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-	1	("6713653").PN.	USPAT; US-PGPUB	2004/06/21 10:47
-	1	("6525192").PN.	USPAT; US-PGPUB	2004/06/24 10:10
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-	35	(low NEAR substituted NEAR hydroxypropyl NEAR cellulose).clm.	USPAT; US-PGPUB	2004/06/24 10:12
-	22	(low NEAR substituted NEAR hydroxypropyl NEAR cellulose).clm.	USPAT	2004/06/24 13:00
-	1	("6495721").PN.	USPAT	2004/06/24 13:00
-	1	("5434295").PN.	USPAT; US-PGPUB	2004/07/08 06:27
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-	11146	(coloring or tinting).clm.	USPAT; US-PGPUB	2004/07/08 10:14
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